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Eruptive flow response in a multi-component driven system by an interacting lattice gas simulation

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Abstract

An interacting lattice gas model is used to study flow of immiscible components A and B (molecular weights M_A and M_B, $M_A < M_B$) by Monte Carlo simulations. Concentration gradients and hydrostatic pressure bias (H) drive these constituents from their source at the bottom against gravitational sedimentation in an effective medium. Response of their flux densities (j_A, j_B) to the hydrostatic bias H are examined. If both constituents are released with equal probabilities (a non-interacting source), their flux densities respond linearly to bias with $j_A > j_B$ except at the extreme bias $H \to 1$ where $j_A \to j_B$. Flow response becomes complex if the constituents from their source are released according to their current lattice concentrations (an interacting source): a crossover occurs from $j_A > j_B$ at low bias ($H \le 0.4$) to $j_B > j_A$ at higher bias ($H > 0.4$). Constituent with the lower molecular weight (A) responds linearly on increasing the bias except at very high bias ($H \ge 0.8$) where the response becomes negative. The heavier component (B) responds non-linearly: a high response at low values of H is followed by a linear response before the onset of eruptive response at high range of H. The volatility parameter diverges as eruption occurs at $H \to 1$.
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1. Introduction

Flow patterns and morphological evolution in the sub-bottom region (at and below) of the ocean floor are complex due to dynamics of interacting components with diverse characteristics such as granular matters (sand, silt, etc.), mixtures of fluids, and gas [1–7]. The response of these constituents to temperature, pressure, and concentration gradients lead to a variety of correlated, local and global phenomena involving flow, extrusion, evolution, and settling of constituents with a range of relaxation time and length scales [4,8–10]. Understanding of structure and dynamics may involve unsteady and steady-state mechanism which are equilibrium and far from equilibrium processes. In particular, studying the flow of methane gas, formation of hydrate, and its dissociation, along with its complex mixtures with other hydro-constituents including

sedimentary compounds has attracted a considerable interest in marine geosciences [9–13]. Of our particular interest are the effects of driving fields such as concentration gradients, hydrostatic pressure, thermal gradient, etc. [14,15] which are crucial in understanding the hydrate formation, mound evolution, and dissociation leading to such instabilities [1] as mud volcanoes [16–18] below the ocean floor.

Enormous efforts [19] have been made in recent years to understand mud volcanoes [20], a violent eruption of mud or clay often accompanied by methane gas. The main cause is believed to be the over-pressure of the fluidized mud (clay, sand, salt water) along with a gas source at depth within the sediment column (due to weight of mud, escaping methane gas, etc.). Most numerical modeling [20] of such complex phenomena involve balancing between the weight and driving pressure and a source of volume flux of simplified systems. Corresponding competing terms offer good estimates of the height reached by the mud volcanoes in the framework of mean-field or first hand analysis. Spatial heterogeneity and local dynamics leading to such cooperative eruption seems to be missing in such study. It would be interesting to develop a model where such a violent global response as eruption appears as a collective cooperative phenomena of its interacting components. Characterizing different components of multi-constituents fluid mixture such as gas, liquid, and sediment by particles with desirable characteristics via coarse grained models seems a viable approach to investigate such driven systems. In a relatively dense system of such mixture, the dynamics of individual constituents and their distribution lead to correlations induced by their interactions. While addressing the global flow is the main issue to address, the underlying self-organizing structural morphology cannot be ignored.

Investigations of structures and patterns in driven granular systems [21,22] have attracted a considerable interests in recent years [23–29]. It is often difficult to monitor the mobility of individual constituents in laboratory experiments [30] in order to understand their global patterns. On the other hand, it is easier to monitor their movements and structural patterns [31,32] by computer simulations such as lattice gas [33,34], molecular dynamics [26,35,36], and Monte Carlo [37] methods. The number of constituents is conserved in most studies of driven particles systems [38,39]. The self-organizing system of our driven mixture is non-conservative where the particles are continuously released from a source (see below). It should be pointed out that it is easier to incorporate interactions between constituent particles and effective medium (empty lattice sites, see below) in interacting lattice gas than that with the Boltzmann lattice gas [40,41].

When an immiscible fluid mixture consisting of two components say, A and B with dissimilar masses (i.e., gas and liquid, oil and gas, oil and water), is released from a source at the bottom (below the ocean floor), several interesting questions arise regarding their flow and structure. How long will it take for constituents to emerge from the top? How does the morphology emerge as their sedimentation occur at different rates? How do they self-organize, mix, or segregate? How can structural evolution and the flow rate respond to an external hydrostatic pressure bias? As pointed out above, understanding such basic questions is essential in context to the flow of methane gas, hydrocarbon, their complex compounds, and hydrate formation and its dissociation below the ocean floor [9–13]. Using an interacting lattice gas model, we have studied [42] the onset of segregation and partial layering in a steady-state flow of an immiscible mixture. Effects of hydrostatic pressure bias (H) and molecular weight ($\alpha = M_B/M_A = 1-10$) on steady-state density profiles have been recently examined and attempts are made to quantify the dependence of their overall density on these parameters (H, α) [43]. Very recently, we studied the response of flux density to hydrostatic pressure bias [44] in a self-organizing immiscible mixture where both components (A, B) are released into the system with equal rate. We observe linear response for both constituents with rates depending on their molecular weights, especially at low bias. We extend this study here to a system where the release of constituents from the source depends on their concentration in the system. Consequently, we find a dramatic change in response of the flux density to bias, from linear to eruptive (see below). The model is described in the next section followed by results and discussion with a summary and conclusion.

2. Model and method

We consider a cubic lattice of size L^3 with $L = 30-200$. Bottom of the lattice ($z = 1$) is connected to a source releasing particles A and B into the lattice. Top of the lattice ($z = L$) is open. Initially, about half of the lattice sites are randomly occupied by A or B with equal probability, the remaining empty sites represent the

background solvent (S). The steady-state global properties do not depend on the initial configuration (see below). Depending on the occupancy ($A, B,$ or S), a lattice site has three states. Our system with mobile particles is characterized by an interaction energy E between these components,

$$E = \sum_i \sum_k J(i,k),$$

(1)

where index i runs over all particles and k over all nearest neighbor sites of i with,

$$J(A,A) = J(B,B) = -J(A,B) = -J(B,A) = -\varepsilon_1,$$

(2)

$$J(A,S) = J(B,S) = -\varepsilon_2.$$

(3)

The miscibility, phase separation between A and B, and their mobility are controlled by ε_1 and ε_2. A positive miscibility gap $\varepsilon_1 = 1$, considered here, enhances the phase separation in contrast to mixing with a negative ε_1. The interaction with the effective host medium is governed by ε_2 which is set at $\varepsilon_2 = 1$. Although these host empty sites appear static, they do exchange their positions with the mobile constituents (see below) and therefore, can be used to vary the viscous drag or the quality of the solvent by varying the interaction ε_2.

Effect of molecular weights of constituents (M_A, M_B) is considered via change in the gravitational potential energy as they move along ($-z$) or against ($+z$) gravity. Further, a hydrostatic pressure bias (H), is also included to drive the constituents upward. The Metropolis algorithm is used to move randomly selected particles to their neighboring sites along $\pm x, \pm y, \pm z$ directions with probabilities,

$$P_x = P_{-x} = P_y = P_{-y} = \frac{1}{6}; \quad P_z = \frac{1+H}{6}, \quad P_{-z} = \frac{1-H}{6}; \quad 0 \leqslant H \leqslant 1.$$

(4)

Change in configurational interaction energy along with the bias, thus, orchestrate the mobility. Periodic boundary condition is used along the transverse direction. Top ($z = L$) and bottom ($z = 1$) of the sample are open for the lattice particles to escape. A particle is released into a bottom lattice site as soon as it is vacated by the particle when it moves up or diffuses laterally.

Two methods are considered to release the type of particles (A or B) from the source: injection probabilities of A and B are equal to their relative concentrations in the lattice in procedure (i) while the probabilities of releasing particles (A, B) are equal in procedure (ii) regardless of their concentrations. Method (i) introduces a stronger interaction between the source and the sample which may be more realistic in many situations, i.e., constituents of a highly viscous fluid have strong attractive interactions in general. Attempt to move each particles once defines unit Monte Carlo step (MCS) time. As the simulation proceeds, the constituents move in and out of the sample. The number of particles and their density profiles (planer densities along x, y, z) evolve but eventually stabilize to a steady-state. Simulations are performed with many independent samples each for a sufficiently long time steps to reach steady-state to estimate the physical quantities reliably. We have observed [32] evolution of interesting structural patterns, i.e., onset of phase separation, oscillation in lateral density profiles, layering etc. which share some characteristics observed in granular systems [26]. In the following, we focus mainly on the global transport and flow.

3. Results and discussion

Simulations are performed on samples of various sizes 30^3 to 200^3 as mentioned above. However, data for most production runs are generated with 30^3, 50^3 and 100^3 lattices using as many as 128 independent runs with largest sample for the entire range of pressure bias $H = 0.0-1.0$. Finite size effects on the qualitative behavior of the physical quantities are negligible particularly with 50^3 and 100^3 samples. We restrict to miscibility gap $\varepsilon_1 = 1.0$, effective medium (viscous) interaction $\varepsilon_2 = 1.0$, molecular weights $m_A = 0.1, m_B = 0.3$, and temperature $T = 1.0$ in appropriate unit of interaction energy and Boltzmann constant. Self-organizing structural evolution leading their steady-state equilibrium has been already examined in depth [42,43] with their different phases, segregation, and mixing.

Transport and mobility of constituents (tracers) can be analyzed by examining the variation of the root mean square (rms) displacements of A and B. Obviously, the particles in the dense phase (toward bottom) are not expected to be as mobile as those in the gas phase (toward top). Most particles entering at the bottom

leave the sample from top in the gas phase. The fast movements in the gas phase dominate the asymptotic dependence of tracers rms displacements on time steps. However, in order to estimate the global transport, it is worth looking at the variation of the rms displacements (R) of the center of mass of each species (A and B) with the time (t) steps. Fig. 1 shows R versus t plots for the various values of bias H. The asymptotic dependence can be described by a power-law,

$$R = Dt^\nu,$$

(5)

where D is a constant and ν, the power-law exponent. For most values of the bias, the overall motion of each constituent (A, B) appears to be drift-like with $\nu \simeq 1$. At extremely low pressure bias, we see the signature of sub-diffusive motion ($\nu < 0.5$ (the diffusion movement)).

Let us examine factors affecting the transport. The stochastic thermal motion (the interplay between the interaction energy and temperature, i.e., diffusion in lateral (transverse) planes) is augmented by three driving fields: (a) the concentration gradient caused by continuous release of particles at the bottom, (b) gravity pulling constituents downward, and (c) the external hydrostatic pressure bias pushing them upward. At low pressure bias, the competition between gravity (downward movement) and the concentration gradient (upward from the bottom), appears to be major cause for the slow transport observed above. Increasing the bias offsets the gravity, leading to a net upward global bias (effect of both concentration gradient and pressure) which drives the constituents into a drift-like motion.

Because of the net driving field along the upward direction, there is a net mass transfer: constituents enter at the bottom and leave mostly from the top (see below). In steady-state, the net amount of components entering the system must be equal to net mass leaving the system, i.e., the conservation of mass leading to the continuity equation. From the variation of the net mass transfer (Q) in time t, we can estimate the current due to mass flow,

$$i = \frac{dQ}{dt}.$$

(6)

The current density (j), current per unit cross-sectional area (A_C),

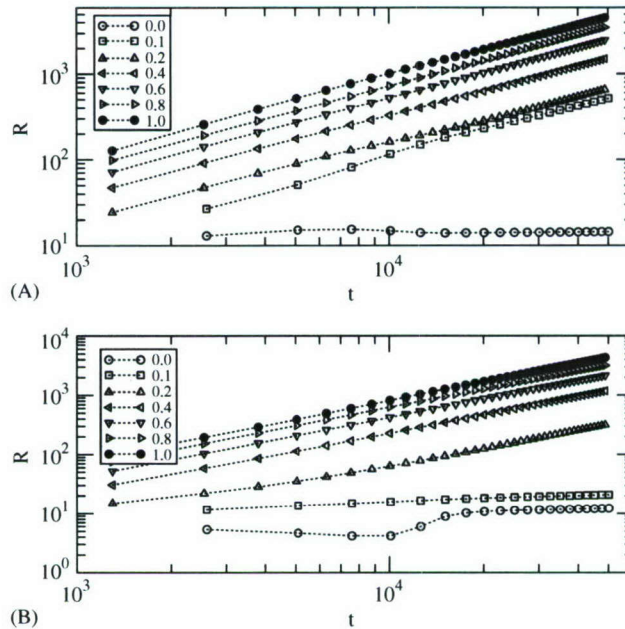$$j = i/A_C.$$

(7)

(A)

(B)

Fig. 1. RMS displacements of the center of mass of A and B versus time t steps at various values of H with $\varepsilon_1 = 1$. Sample size 100^3 with 64–128 independent runs are used.

In presence of a field Δp (pressure, flow field, concentration, etc. and their combination), one may expect, at least in simple cases, a power-law dependence,

$$j = \sigma(\Delta p)^{\beta}, \tag{8}$$

where σ is an analog of conductivity. The exponent $\beta = 1$ corresponds to the well-known Darcy's law of linear response. In our case, it is rather difficult to estimate Δp due to different driving mechanisms mentioned above. However, we can examine our data to extract the response of j to pressure bias (H), the variable in our study.

According to conservation of mass (continuity equation), the flux current density (j) must be independent of time in the asymptotic regime. Fig. 2 shows the temporal variation of j for B (heavier) constituents (similar asymptotic behavior is also observed for A constituents). We see that the flux densities at both bottom and top become equal after an initial relaxation time and remain constant thereafter. The current density depends on the pressure bias (H). Variations of j_A and j_B of constituents A and B, respectively, with H are presented in Figs. 3 and 4. A linear response is generally seen in both systems, i.e., with concentration dependent (i) (Fig. 3) and independent (ii) (Fig. 4), for most region of H which implies the validity of the Darcy's law. When constituents A and B are released with equal probabilities (ii), their respective current densities (j_A, j_B) respond linearly to nearly entire range of bias H (i.e., $\beta \simeq 1$); the prefactor σ is larger for the heavier component (B). The response of current density for system (i), on the other hand, is much more complex. The flow of A responds differently than that of B as expected due to difference in their molecular weights. While the flow density j_A of constituents A is larger than j_B at lower bias ($H \leqslant 0.4$), the flow of constituents B becomes larger than that of A, i.e., $j_A < j_B$, at higher bias ($H \geqslant 0.4$). Since B has larger molecular weight, they tend to gravitate more than A toward the bottom. As a result, particles B have higher probability of leaking from the bottom than particles A particularly at lower bias. Increasing the upward bias (H) reduces the effect of gravitation which results in a larger j_B. Relatively larger amount of B constituents enter the sample at larger H. Thus, the competition between gravity and hydrostatic pressure bias, leads to the crossover from A dominated flow ($j_A > j_B$) at lower bias H to B dominated flow ($j_A < j_B$) at higher H.

At extreme values of bias, the response becomes non-linear with a rapid increasing response of B leading to a "eruptive flow". At the same time, the flow response of A becomes non-monotonic with a rapid decay of j_A
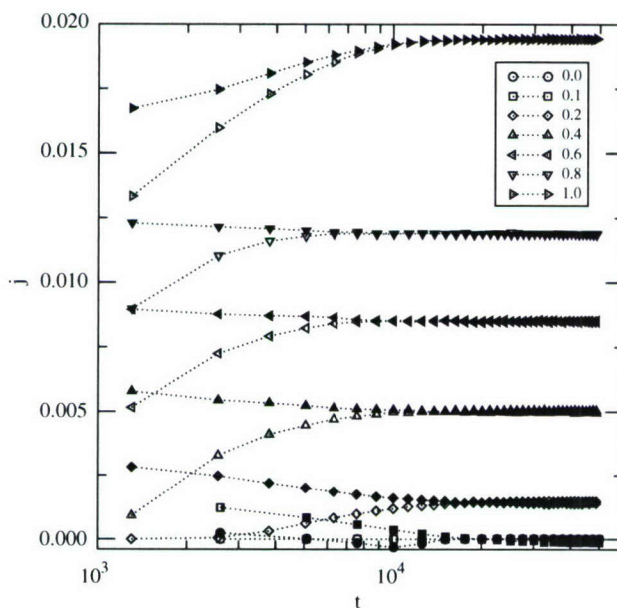

Fig. 2. Flux density j of B from top (open) and bottom (filled) with time steps for the same parameters as in Fig. 1.

Both systems (i) and (ii) are open for constituents to escape. There is a net flow of mass of these immiscible constituents (A, B) without conserving their concentrations. However, steady-state density profiles are obtained and the continuity equations for the conservation of mass of each components are satisfied within the range of statistical fluctuations. If the release of particles from the source is independent of their concentration, we find that corresponding current densities (j_A, j_B) respond linearly to bias (H). Further, $j_A > j_B$ except at extreme value of H ($\to 1$), $j_A \simeq j_B$. In system i where the reservoir and the lattice are correlated with a concentration dependent release rate of constituents, the flow response is complex. We observe a crossover in response of the current densities from low region of bias ($H \leqslant 0.4$) with $j_A > j_B$ to higher range of bias ($H > 0.4$) with $j_A < j_B$. Constituents (A) with lower molecular weight respond linearly to bias for most region of H except at high values ($H \geqslant 0.8$) where the response becomes non-monotonic. The heavier component (B) responds nonlinearly on increasing the bias: a large response at low values of H followed by linear response before an vulcanizing response in high range of H. We have defined a volatility response parameter V_B which seems to diverge $V_B \to \infty$ as $H \to 1$; corresponding parameter for A becomes negative in this range.

In summary, we have identified the linear response region of both immiscible components (A, B) where Darcy's law is valid and provided empirical relations. Differences in response of two immiscible components depending on their molecular weight are identified in two systems of source reservoirs. We are able to identify the condition in which an eruptive flow response occurs which may complement existing modeling [20] and stimulate further interest in this field [19].

Acknowledgments

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